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19. Our chief concern is the production of a STO (Slater-type orbital) integral package with application to diatomic and polyatomic molecules and ions by use of the "Columbus Codes". Comparisons are to be made with GTO (Gaussian-type orbital) codes. We feel confident that the superiority of STOs over GTOs will be most pronounced for excited states and multiple moments using inverse powers of the radial distance. Our judicious use of integer arithmetic and expansions in Taylor series should bring success to the elusive goal. The outline of this new strategy is presented in a recent paper: "Analytical Evaluation of Multicenter Molecular Integrals Over Slater-Type Orbitals Using Expanded Lowdin Alpha Functions". Work on electron scattering continues to move at a rapid pace. The finite difference method has gained international recognition with Dr. Weatherford's presentation of his results at a conference in Italy and the presentation at the ICPEAC meeting in London by his collaborator, Dr. Temkin. Naturally, we hope to combine this method with STOs.

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Submitted by H.W. Jones and C.A. Weatherford
Florida A&M University
Tallahassee, FL 32307
Tel.: (904) 599-3470

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PAPERS PUBLISHED AND WRITTEN

1. H.W. Jones, "Exact formulas and their evaluation for Slater-type orbital overlap integrals with large quantum numbers", Phys. Rev. A, 35, 1923 (1987).

2. H.W. Jones, B. Bussery, and C.A. Weatherford, "An E-Matrix for the Löwdin Alpha-function, Expanded in a Taylor Series: An Analytic Treatment of Molecular Charge Density Near the Origin", Int. Journal of Quantum Chem. 21, 693 (1987).

3. H.W. Jones, Progress Report. "The Exponential Integral Function Ei Computed to Specified Accuracy".

4. C.A. Weatherford, F.B. Brown, and A. Temkin, "Inclusion of Electron Correlation for the Target Wave Function in Low to Intermediate Energy e-N_2 Scattering", Phys. Rev. A, 35, 4561 (1987).

5. C.A. Weatherford, "An Analytic Method for the Three-center Nuclear Attraction Integral: A Generalization of the Gegerbauer Addition Theorem", Int. Journal of Quantum Chemistry 33, 19 (1988).

6. H.W. Jones, "Analytical evaluation of multicenter molecular integrals over Slater-type orbitals using expanded Löwdin alpha functions, Phys. Rev. A, 38, 1065 (1988).

7. H.W. Jones, B. Etemadi, C.A. Weatherford, "Analytical Evaluation of the Electrostatic Potential for Diatomic Molecules", Int. J. Quantum Chem. (To be published).